Development of a CFD Model for Natural Gas Engine Knock

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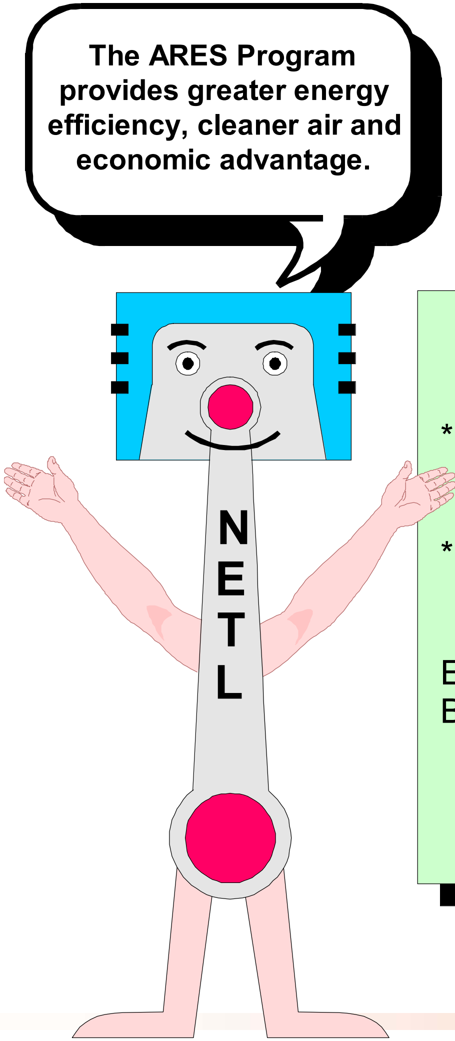
Partner: Fluent, Inc.

Research Objective

- **Objective**
  - Develop a commercial CFD tool for analysis of engine knock.
- **Technical Approach**
  - A knock model will be developed and validated using literature data and engine experimental data and implemented into a commercial computational fluid dynamic software package.

ARES Overview: Program Benefits



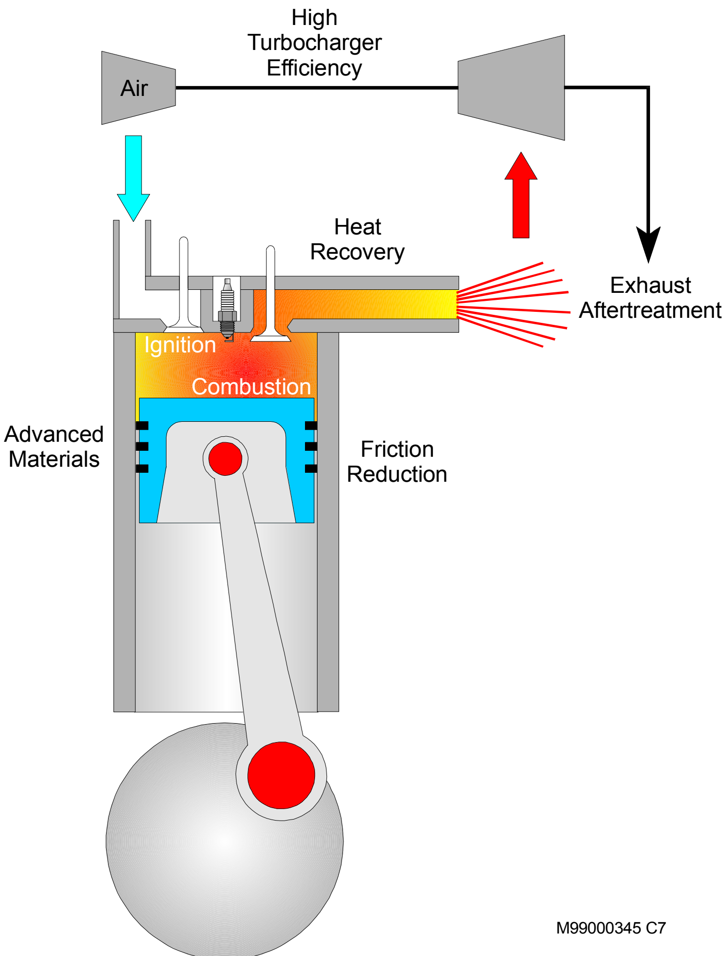
Benefits

	Improvement		Outcome
	From	To	
*Efficiency	38%	50%	- Savings of $320M/yr in fuel cost - Reduction of 8-12M tons/yr CO_2
*Emissions NOx	1 g/bp-hp →	0.05 g/bp-hp	- Reduction of 40,000 - 60,000 tons/yr NOx

Economic Benefits: Will provide domestic engine manufacturers the leverage to compete against foreign manufacturers in this the expanding U.S. Distributed Generation and World

* Assumes 25% market penetration in 300-3000kW range in current NG receprocating Engine Market

ARES Overview: Technology Requirements



✓**Ignition** targets the issues with spark plug wear and lean-burn combustion limits in natural gas engines.

✓Advanced **Combustion** methods are needed to achieve the target low NOx emission and high efficiency levels and **especially a widened knock margin. Focused efforts are needed on computer modeling and simulation of advanced concepts.**

✓**Advanced Materials** are projected to be an important element of the ARES program for applications in demanding high-temperature designs and components.

✓**Advanced Sensors and Controls** will be needed as part of a next-generation system for engine controls to meet the aggressive emissions and efficiency targets. New exhaust emission sensors for NOx, in-cylinder pressure measurement, dynamic torque sensors, advanced engine diagnostic strategies are examples of key components.

✓**Exhaust Aftertreatment** is a key element of achieving the low emission targets. Development of specific catalysts for these engines will be one of the most significant challenges. Spin off technologies will benefit other stationary and mobile applications.

✓**Heat Recovery and Friction Reduction** have shown to be two very important issues from recent engine modeling by Southwest Research Institute and the ARES Engine Consortium. Novel coatings that reduce ring pack friction and reduce heat transfer to engine liner and piston will be investigated.

Past work

- **Prior investigations**
  - Resulting pressure waves breakdown boundary layer resulting in increased surface temperatures creating undesirable material response. Knock is Bad!
  - High potential payoff in efficiency for increased brake mean effective pressure (BMEP) resulting from improved knock resistance **Need higher efficiency!**
  - Optical studies indicate significant increases in specific radical species during and prior to the knocking phenomena **Novel stuff is happening leading to knock!**
  - Threshold pressures required in end-gas for knock initiation **Reduce P, Increase flame Speed**
  - Ignition delay of natural gas highly dependent on detailed mechanism of C3 and higher hydrocarbons **Proper chemistry is important in modeling**
  - Liquid fuels (gasoline) used in overwhelming majority of previous work

Model Development -<u>Approach</u>

- **Develop modeling tool to accurately predict knock in ARES engines - attempt to independently validate kinetic and fluid mechanisms**
  - Kinetic Mechanism Development
    - Search for best reduced mechanism
    - Compare to Full GRI Mech 3.0
  - CFD Platform
    - **Fluent 6.X <u>(Final product = User friendly CFD model for knock prediction)</u>**
  - Validation
    - Use KIVA with full mech “Can we see knock?”
    - Use available data from the literature to validate Fluent
      - Nabors et al., (dfaf), Methane jet, kinetic/fluid coupling undesirable
      - Lee et.al., (dfsd), simple H_2 chem., experiments well characterized
      - Brett et. al., (2001), RCM data, limited experimental detail
    - Use NETL reciprocating engine as validation tool

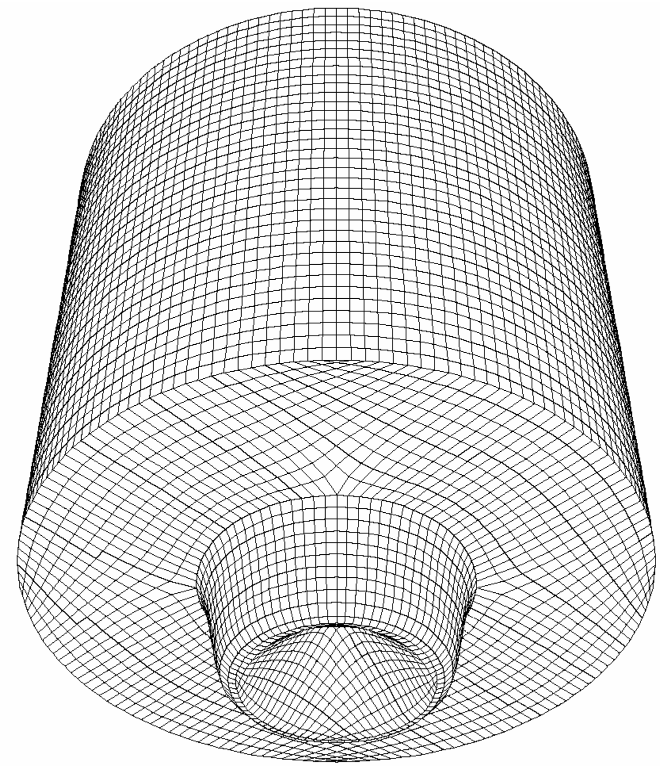
Model Development

Work-to-Date: Kiva, Full Mechanism

3-D simulation:

Homogeneous charge, Fuel = Methane

- CR = 25, Bore = 86 mm, Stroke = 75 mm, Squish = 1 mm; 1500 RPM
- A/F = 17.03; equivalence ratio = 1.0
- Ignition = 26° CA BTDC
- Diesel geometry



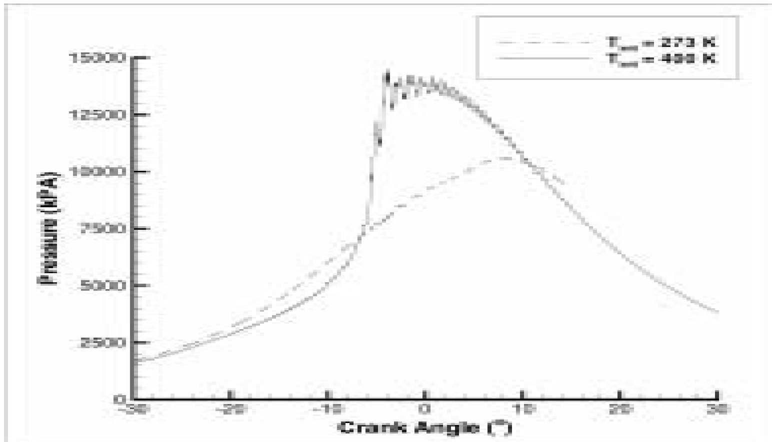
– k-ε subgrid-scale turbulence model
– Partially stirred reactor model with three time scales, t_{mix}, t_{chem}, t_{res}

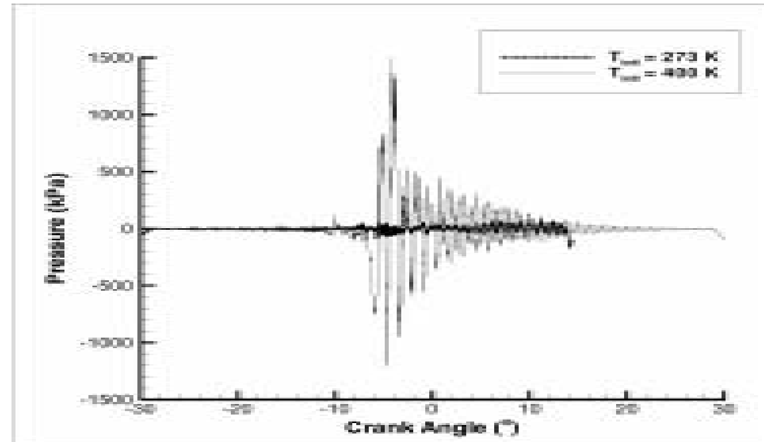
– Detailed DME (di-methyl ether) chemistry with CH_4 sub-mechanism: 135 reactions, 33 Species.

Model Development

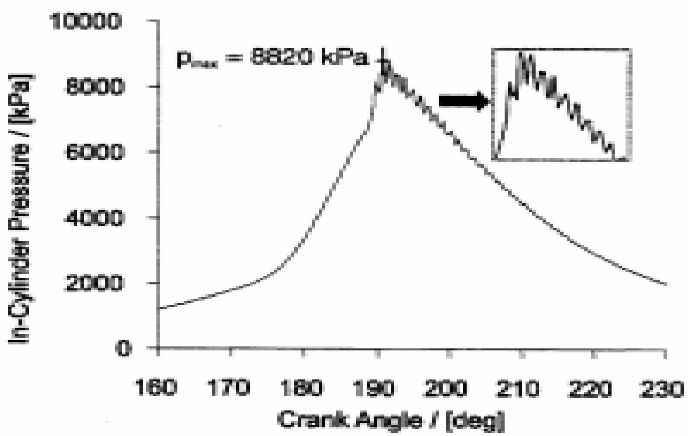
Work-to-Date: Kiva, Full Mechanism

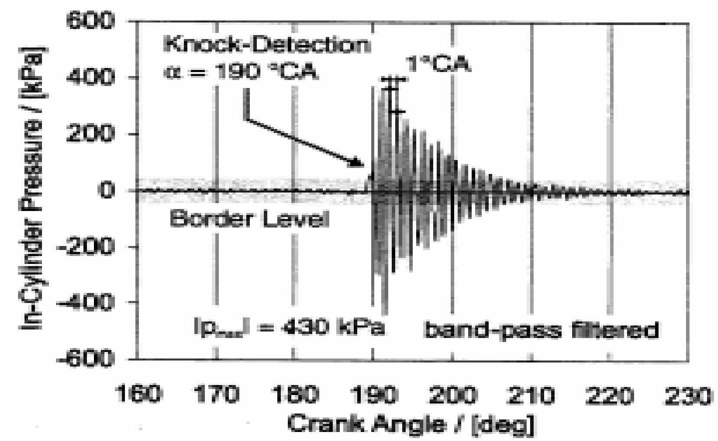
- Pressure variations (4-14 KHz) (predicted, 3-D)



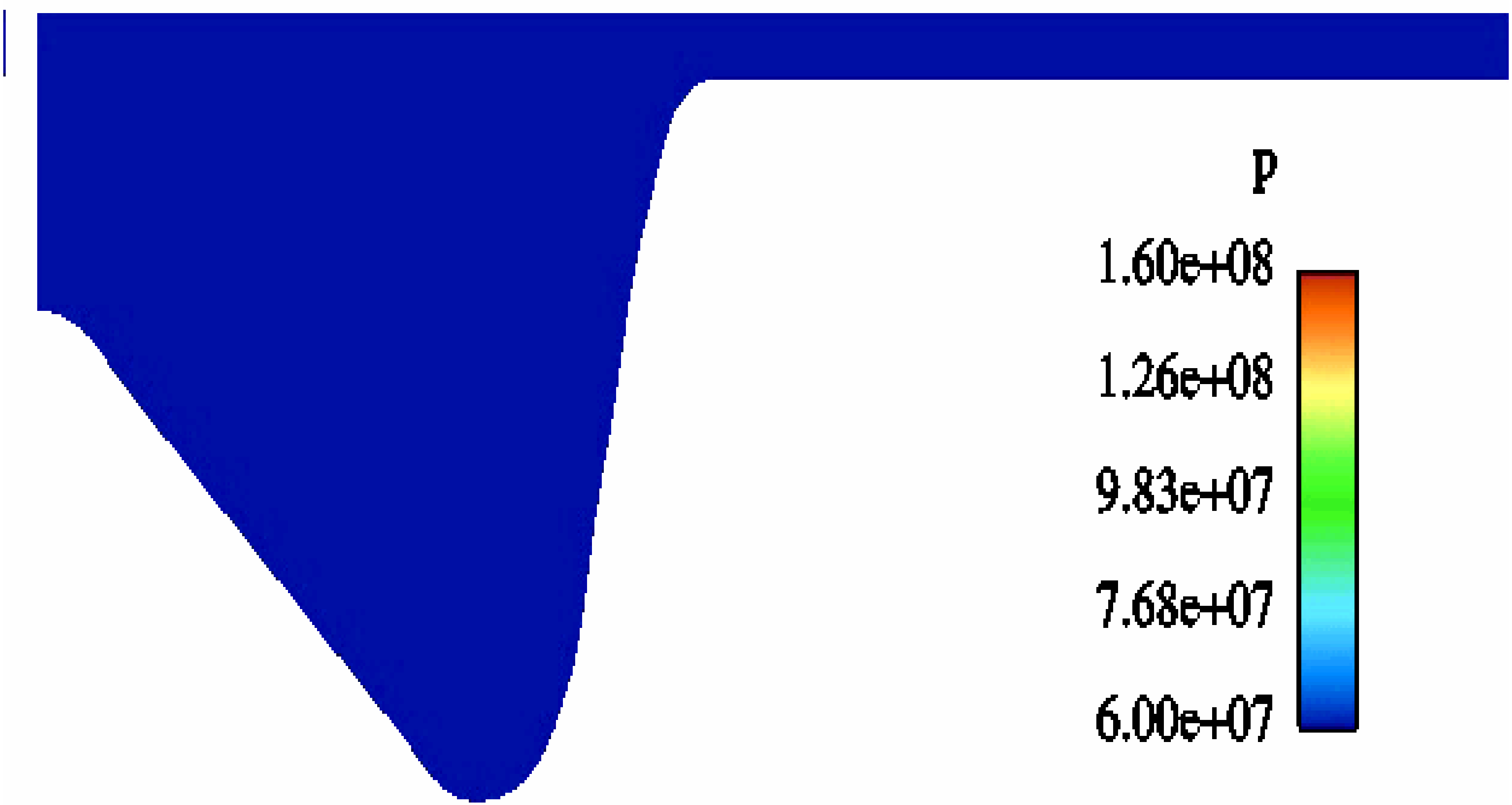


- In-cylinder pressure data (band-pass filtered f= 4 - 14 KHz) (Toepfer et al.,2000)



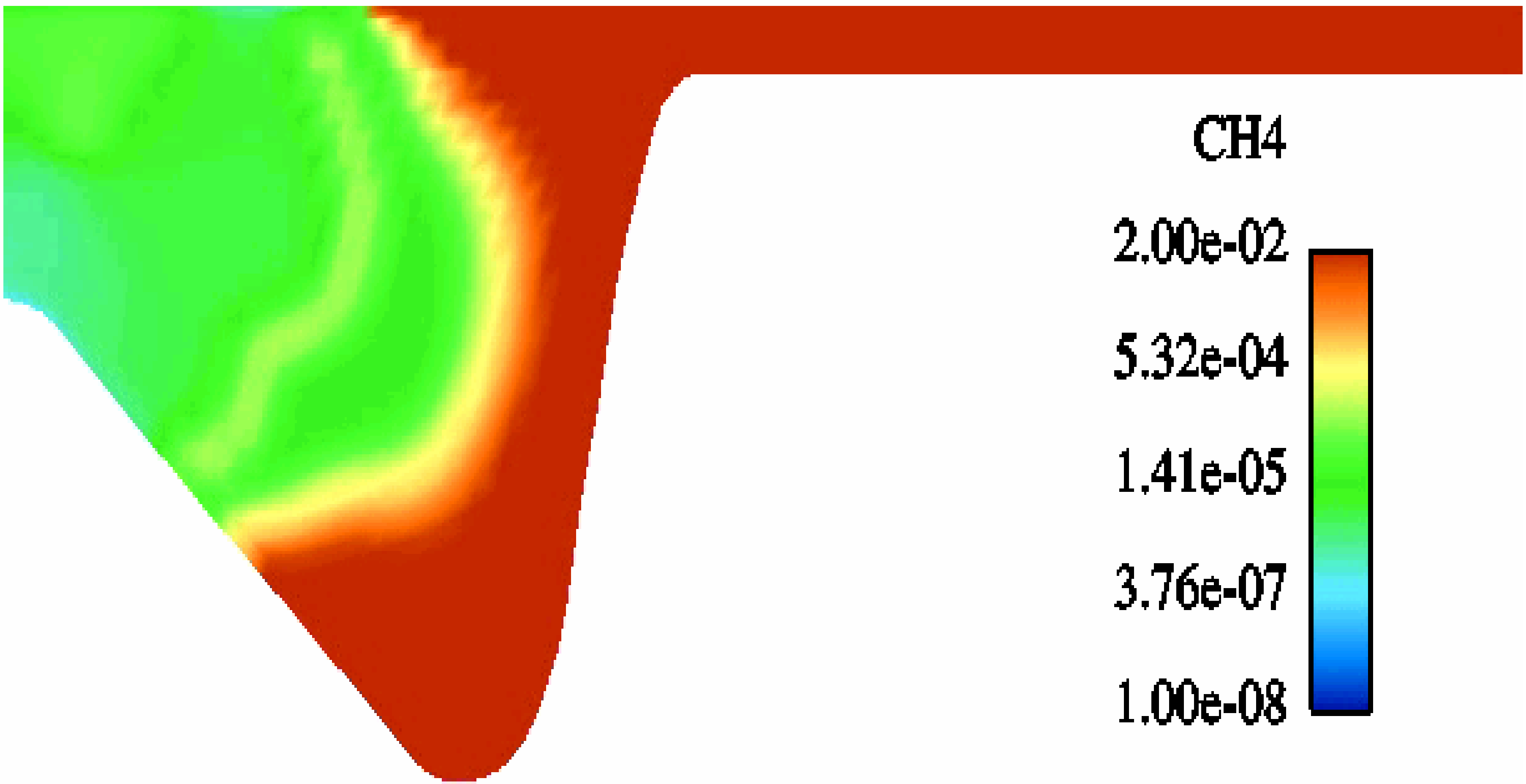


Model Development
Work-to-Date: Kiva, Full Mechanism



Model Development

Work-to-Date: Kiva, Full Mechanism



Model Development

Work-to-Date: Fluent Model of Nabor et al.

- Ignition model in FLUENT CFD code is used to simulate Naber et al's experiment with natural gas in a pre-heated and pressurized combustion bomb.

- Reduced GRI-Mech DRM19 and DRM22 chemical kinetic mechanisms are used in conjunction with chemical kinetics code Chemkin for this study.

- DRM19 consists of the following active species plus nitrogen (H_2, H, O, O_2, OH, H_2O, HO_2, CH_2, CH_2(s), CH_3, CH_4, CO, CO_2, HCO, CH_2O, CH_3O, C_2H_4, C_2H_5, and C_2H_6). Methane gas break up is modeled using 84 elementary reactions

- DRM22 includes of all the species of DRM19 plus C_2H_2 , C_2H_3 , and H_2O_2. Methane break up is modeled using 104 elementary reactions.

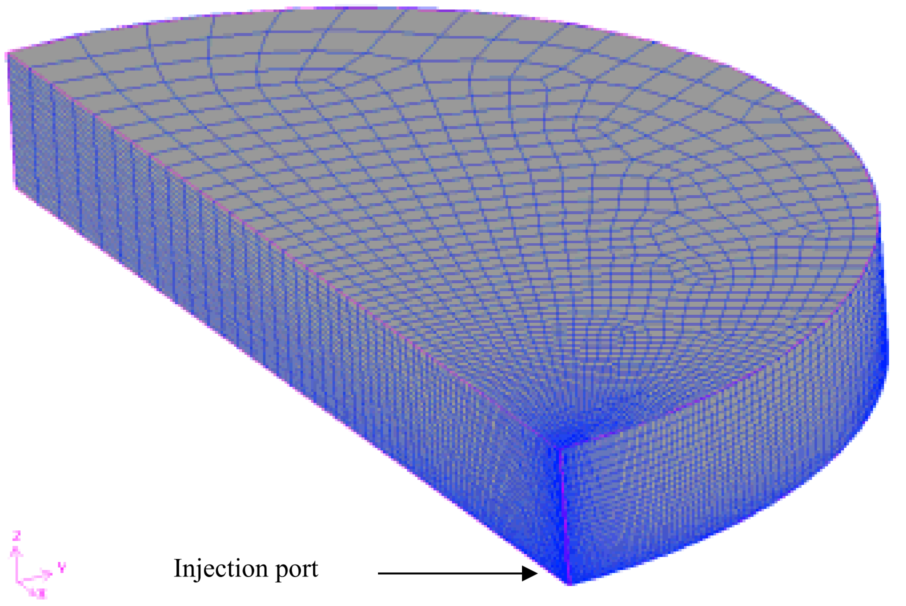
Model Development

Work-to-Date: Fluent Model of Nabor et al.

Combustion vessel used in Naber et al's work has a diameter of 114 mm and a width of 28.6 mm. A single fuel injector which has an orifice diameter of 0.25 mm injects fuel toward the center of the vessel.

- Pure methane and two other blend of natural gas are injected into vitiated air at temperatures of 1500, 1400, 1350, 1300, 1200, and 1100 °K and a vitiated air density of 20.4 kg/m^3 (6.9 atm@1200K)

- Ignition delay is defined by Naber's et al as the elapsed time from start of fuel injection to the time when a net pressure rise of 14 kPa is measured in the combustion vessel.



Model Development

Work-to-Date: Fluent Model of Nabor et al.

Temperature (^{o}k)	Methane		
	Naber et al.[2]	Naber et al.[1]	DRM19 prediction
1200	1.15	1.80	4.12
1300	0.61	0.92	1.09
1400	0.48	0.60	0.492
1500	0.41	0.50	0.524

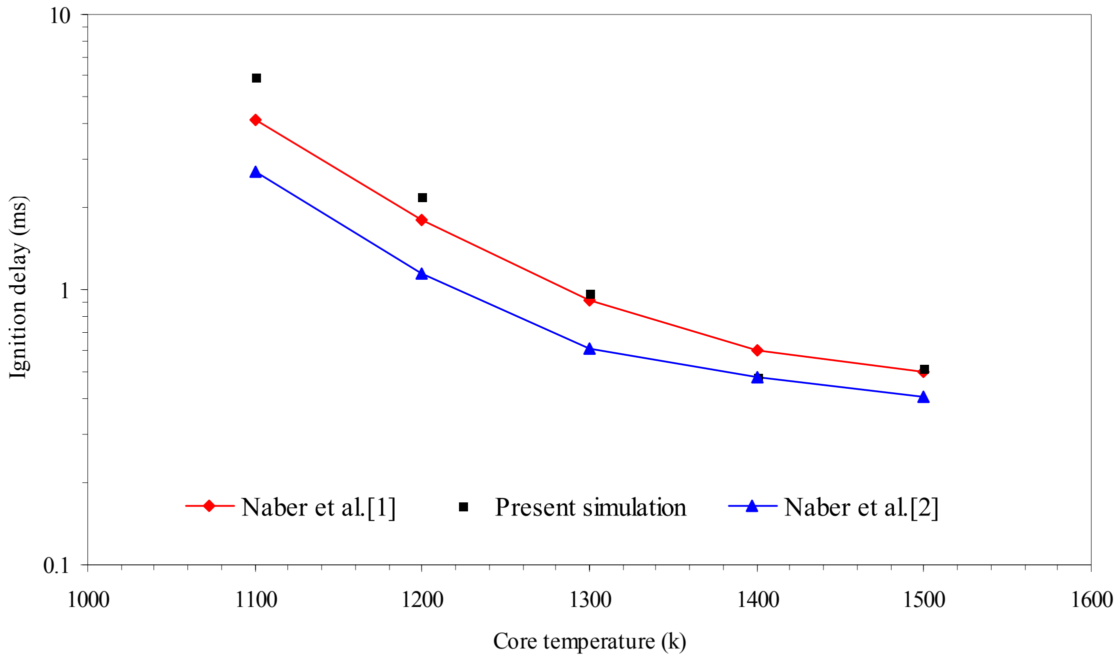
- DRM19 overpredicts the ignition delay in particular at vitiated air temperature of below 1200 ^{o}K. Ambient density 20 kg/m^3 (6.9 atm @1200K)

Core Temperature (^{o}K)	Present simulation (ms)	Naber et al.[3] measured data (ms)	Naber et al.[9] measured data (ms)
1100	5.91	2.70	4.15
1200	2.16	1.15	1.80
1300	0.976	0.61	0.92
1400	0.482	0.48	0.60
1500	0.32	0.41	0.50

- DRM22 has additional C_2 chemistry (i.e. C_2H_2 and C_2H_3), which important for oxidation of methane. Moreover, DRM22 includes H_2O_2 which is an effective ignition promoter for natural gas.

Model Development

Work-to-Date: Fluent Model of Nabor et al.



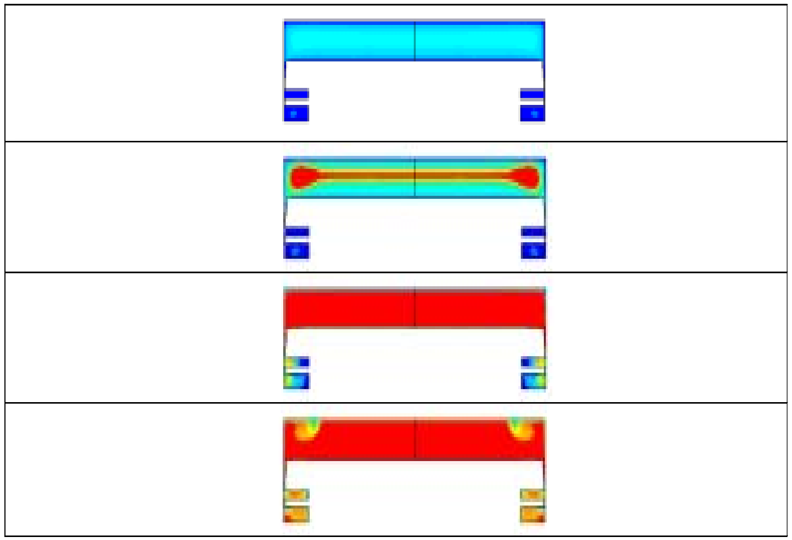
•Ignition delay for pure methane as a function of ambient air temperature for ambient air density of 20.4 kg/m^3 using DRM22.

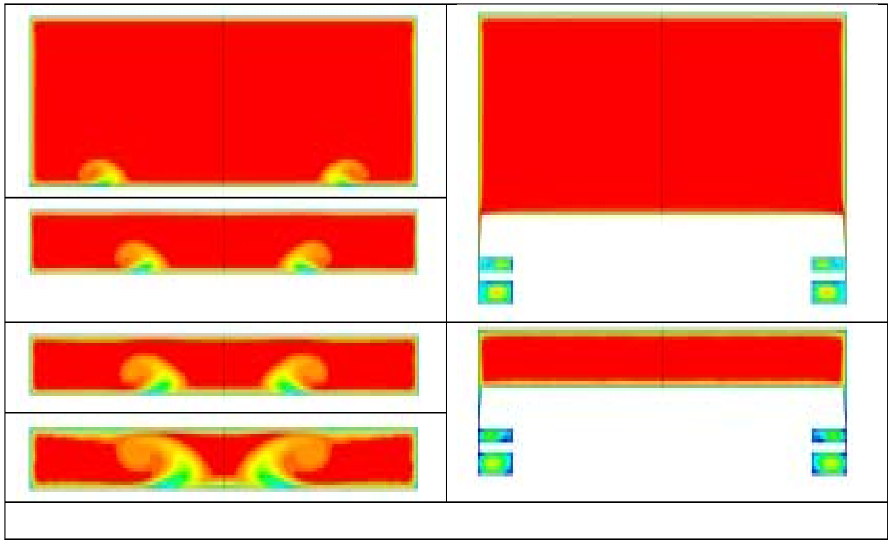
References

1. Naber, J.D., Siebers, D.L., Di Julio, S.S., and Westbrook, C.K.,"Effects of Natural Gas Composition on Ignition Delay Under Diesel Conditions", Combustion and Flame, 1994.

2. Naber, J.D., Siebers, D.L., Caton, J.A., Westbrook, C.K., and Di Julio, S.S., "Natural Gas Autoignition Under Diesel Conditions:Experiments and Chemical Kinetic Modeling", SAE Technical Paper 942034, 1994.

Piston Geometry Affects Temperature Profile

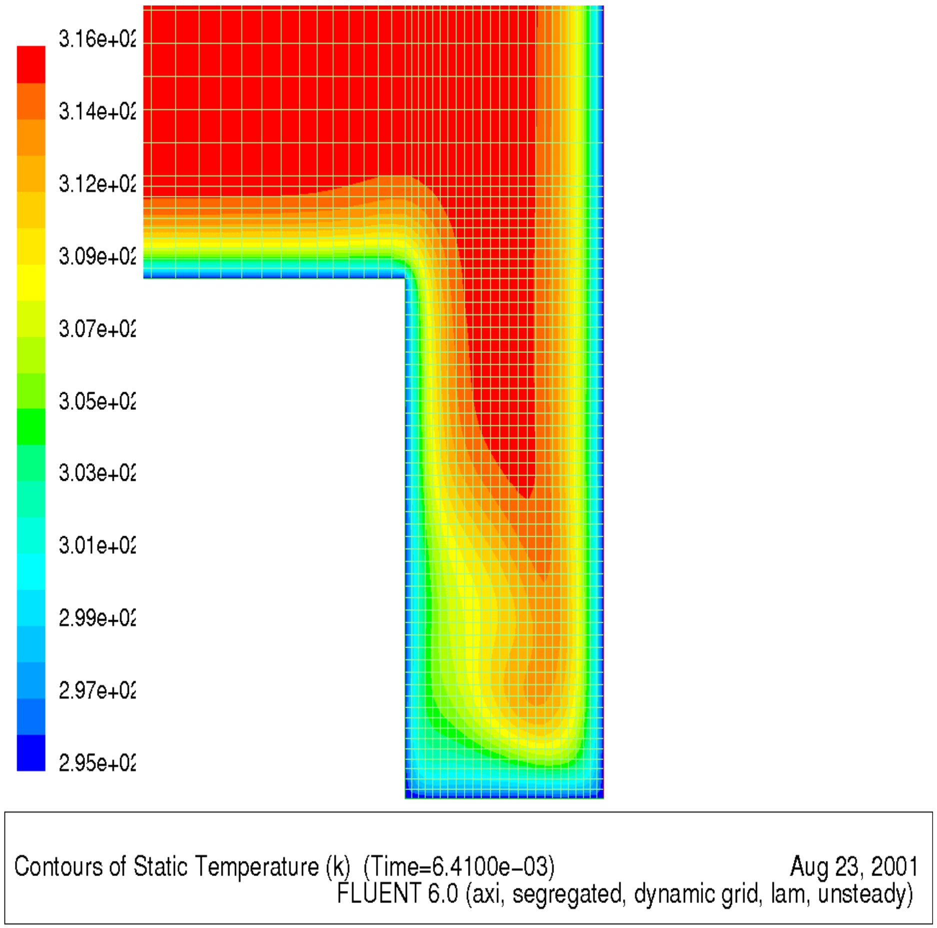


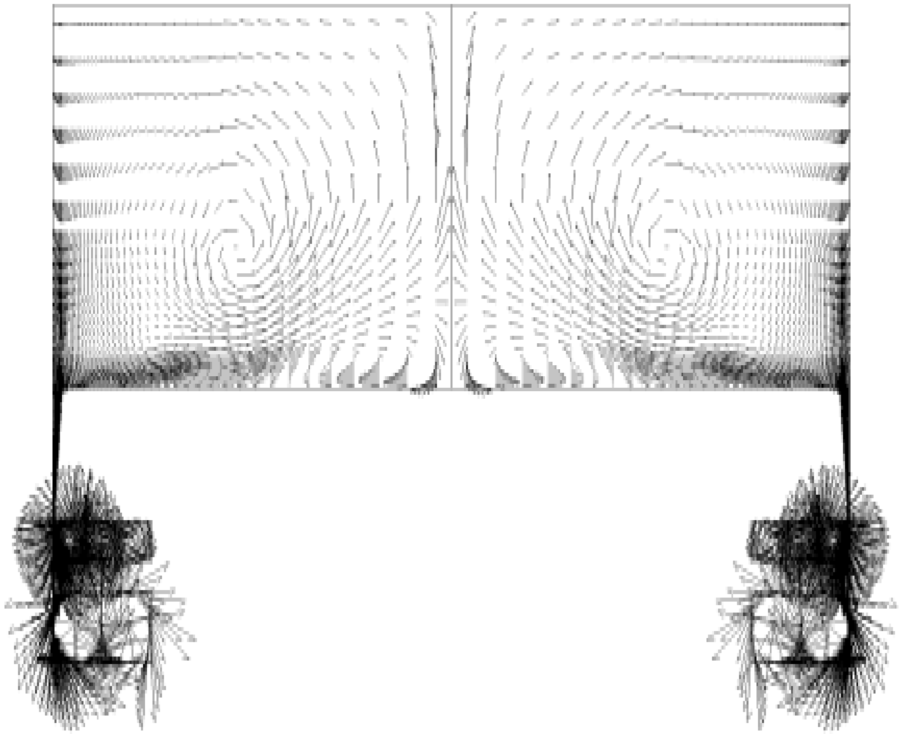


Temperature contours are shown above immediately before and after ignition. The top image shows that, near the wall and in the crevice region, the temperature is lower than the core due to heat transfer. As indicated by the high temperatures, ignition occurs in the central core of the chamber (second image). The bottom image, which is taken some time after ignition, shows that the combustion front propagates into the crevice region and forces the low temperature crevice gases out into the main chamber.

The effect of the piston shape on the vortex roll-up can be seen in Figure 23 for a non-reacting case. This figure displays a sequence of temperature contours immediately before and after the end of compression for both a flat (left images) and creviced piston (right images) heads. As can be seen, the piston rollup is significant for the flat piston. The temperature difference between the core and the center of the vortex is over 200 K. This roll-up is not seen with the creviced piston. The core temperature is uniform with a sharp gradient near the fixed temperature walls.

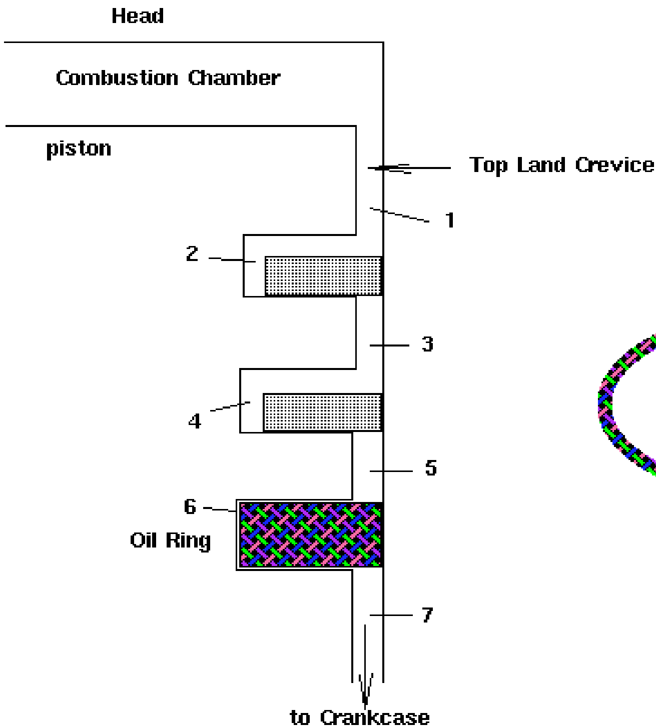
Crevice Velocity/Temperature

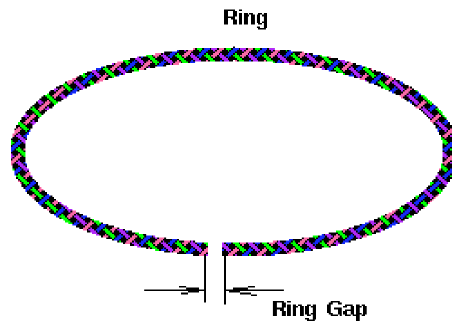


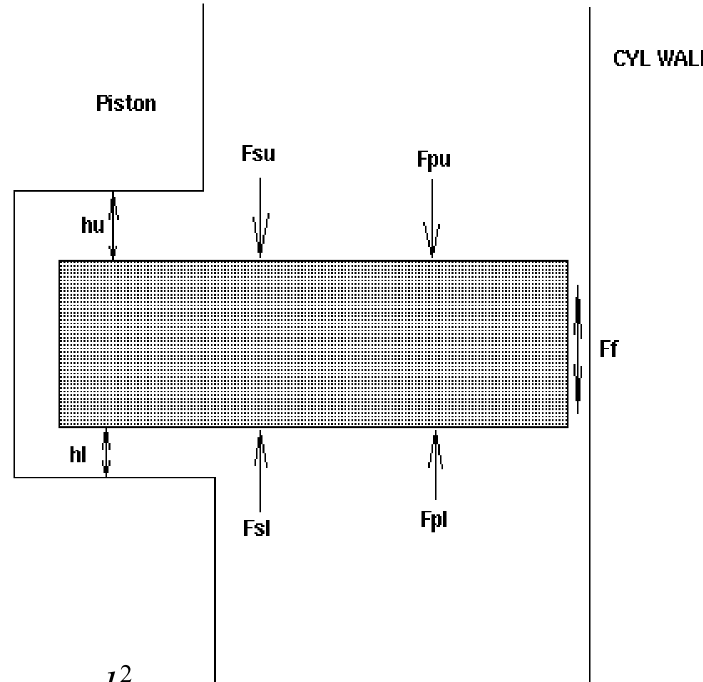


NETL

Ring Crevice Model







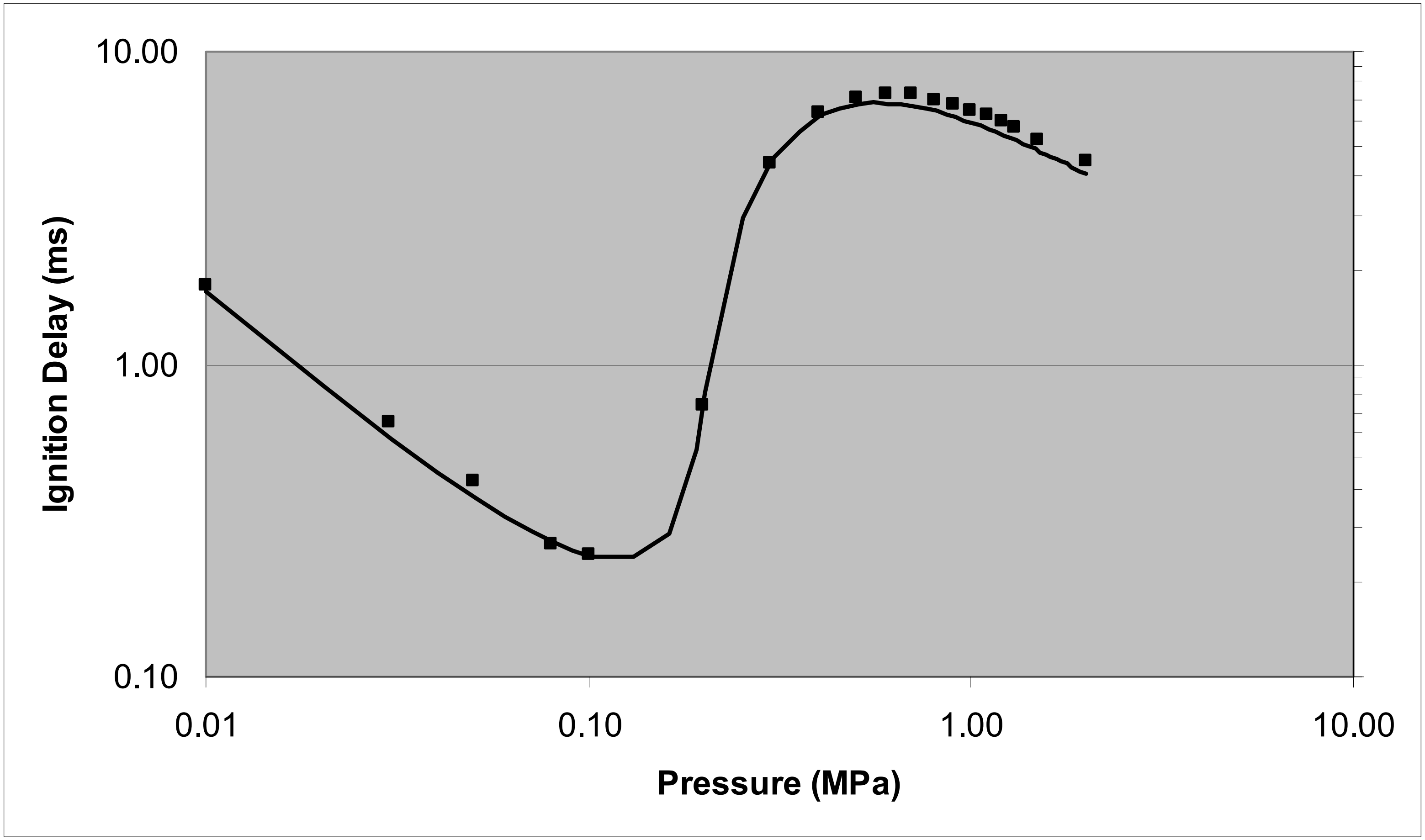
$$\frac{dP_2}{dt} = \frac{P_2}{m_2}(m_{12} - m_{23})$$

$$m_r \frac{d^2x}{dt^2} = F_{sl} - F_{su} + F_{pl} - F_{Pu} - F_f$$

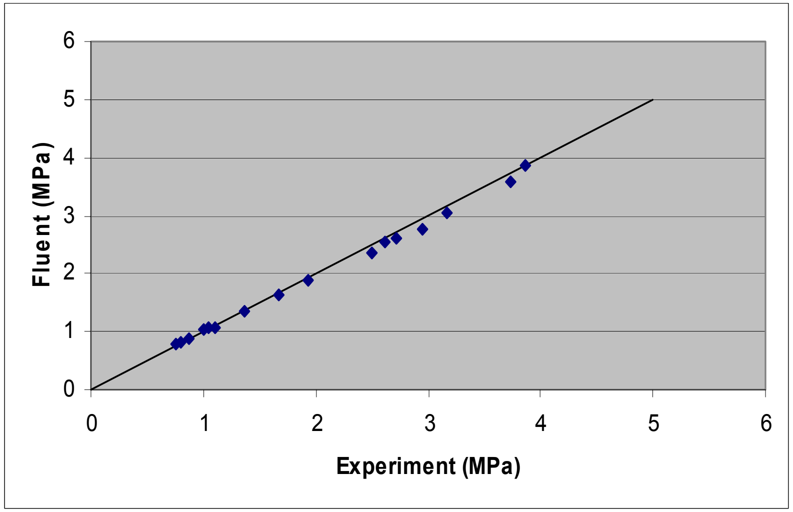
$$\frac{dh_l}{dt} = V_r - V_p = -\frac{dh_u}{dt}$$

$$\frac{d^2x}{dt^2} = \frac{dV_r}{dt}$$

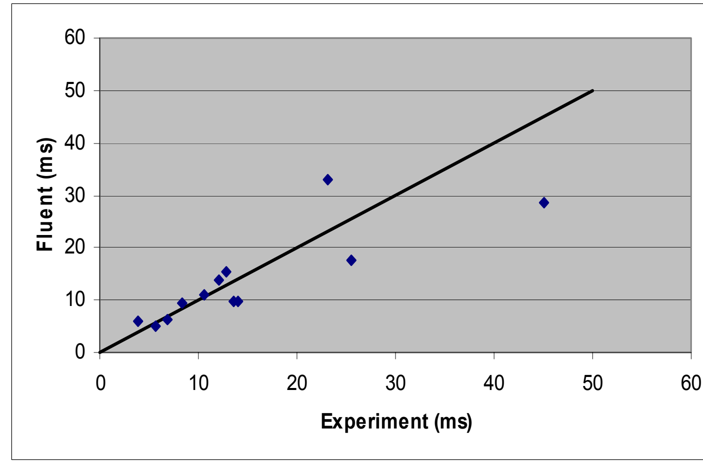
Ignition delay as a function of pressure ($H_2/O_2/Ar$ mixture, adiabatic) predicted by Senkin (symbols) and Fluent (line)



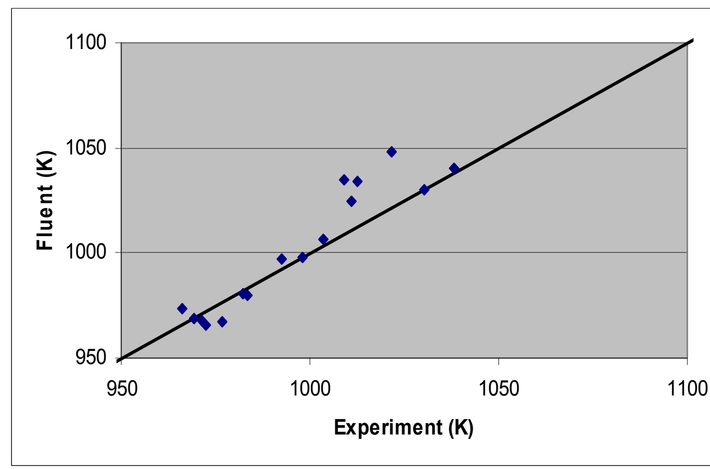
Fluent vs. Experimental H_2 Combustion



Peak Pressure



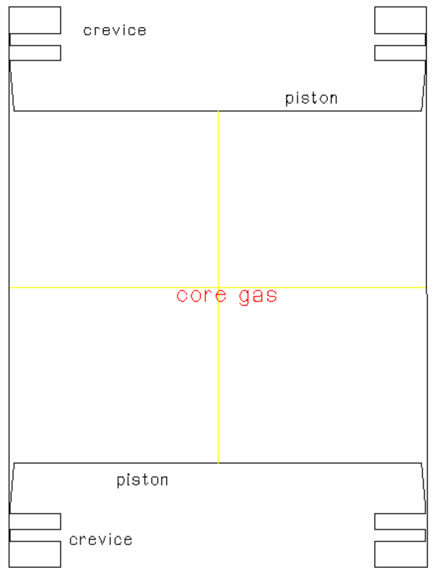
Ignition Delay



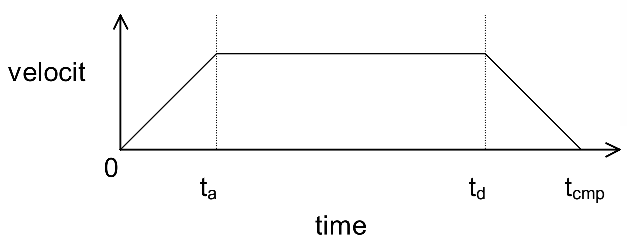
Peak compression temperature

- **RCM data from Lee and Hochgreb, 1997/1998**
- **Kinetic Mechanism from Kim et al., 1994**

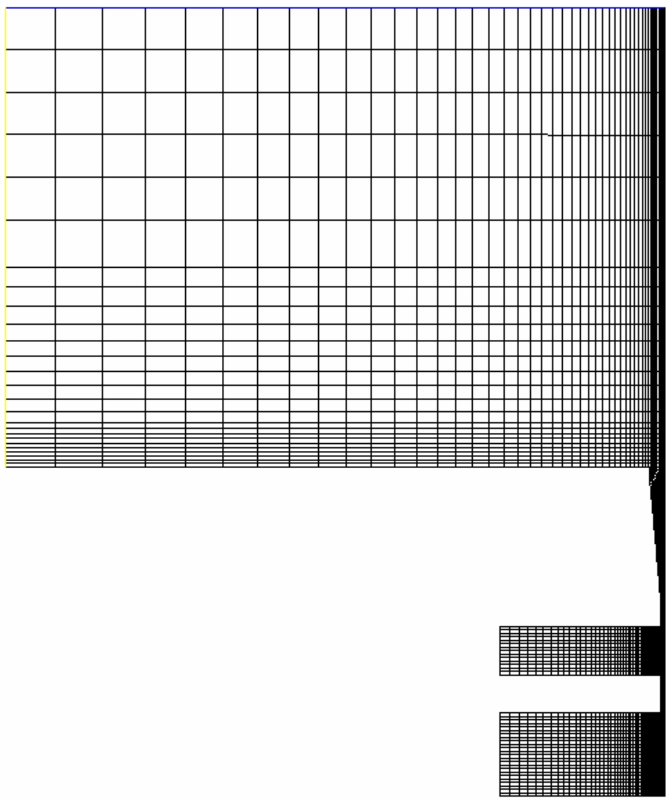
Experimental Setup for Brett et al.



Schematic of RCM cylinder

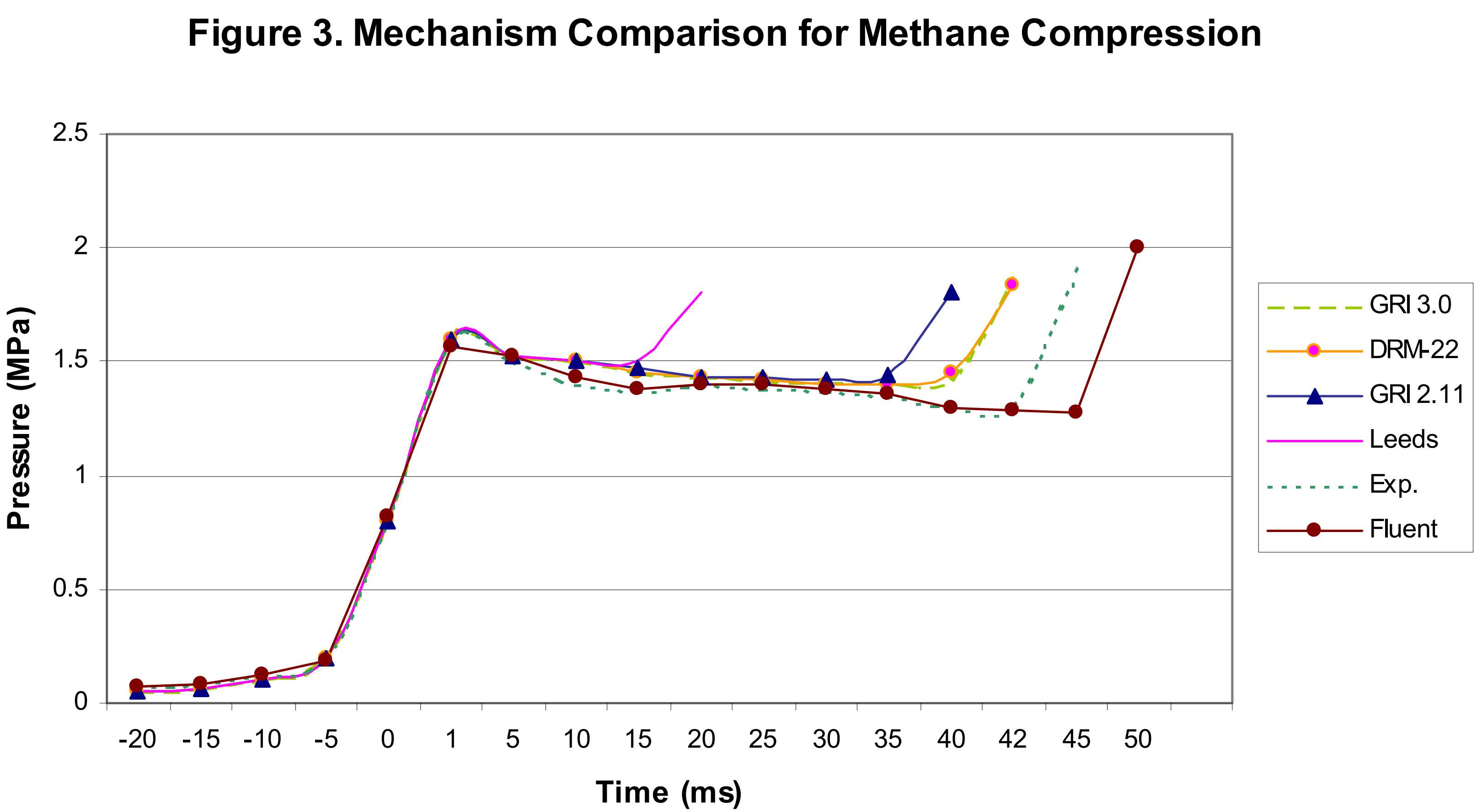


Piston Velocity Profile

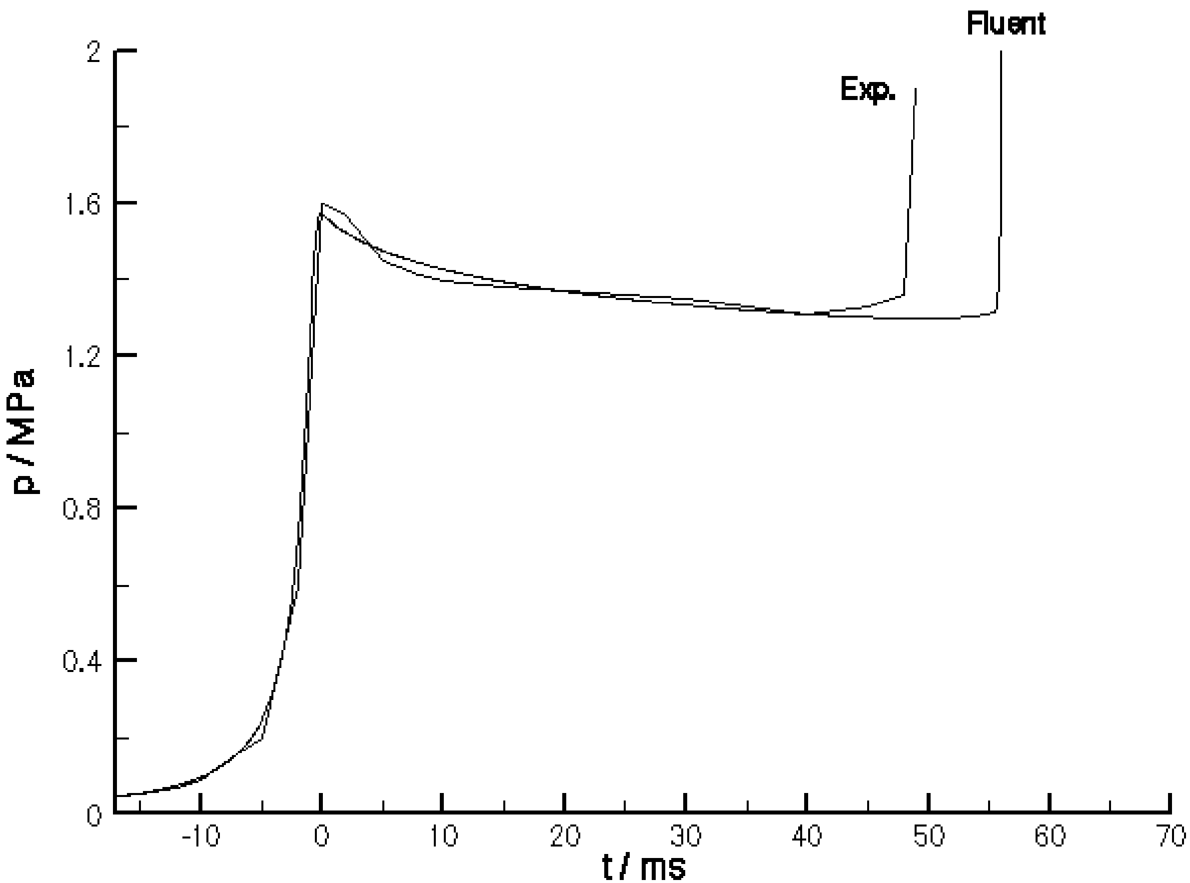


Computational Mesh

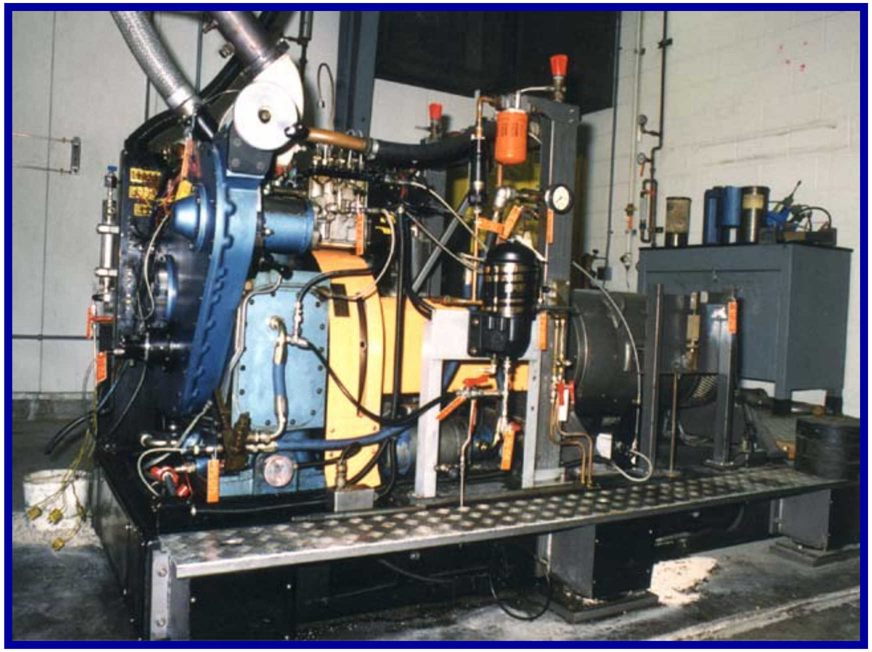
Methane Compression (Chemkin/Senkin)



Comparison to (Brett et al., 2001) Methane



Engine Validation Test Bed



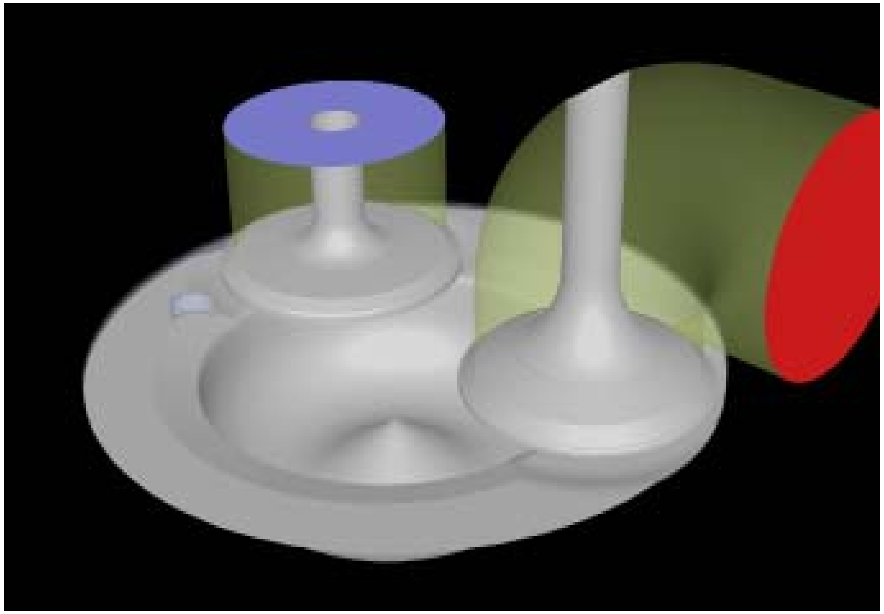
Bore: 130 mm (5.1 in.)

Stroke:150 mm (6.0 in.)

CR: 13.3:1

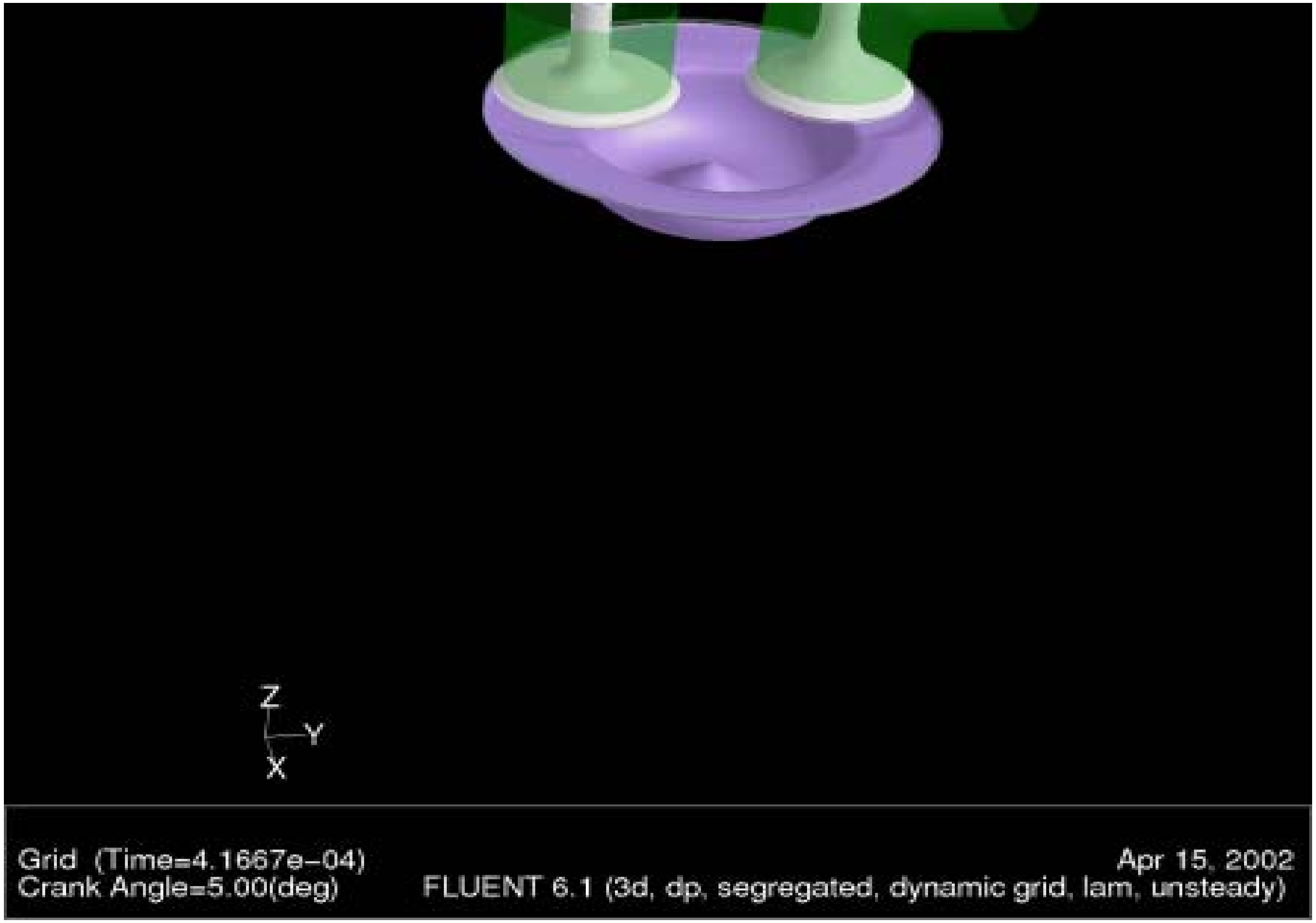
Output: 55KW (74 hp) @ 2200 rpm

FIE: Bosch A700 PLN, 3850 psi NOP



Ricardo Proteous Single-Cylinder 2-liter, direct-injected Diesel Engine

NETL Engine - Moving Mesh - Fluent 6.1



Present Status

1. Validated autoignition models for methane.

2. Discovery of the influences of the chemistry and flow field on the autoignitions.

- Convenient pre-process for Fluent: setting up the detailed chemistry kinetics by using Chemkin type input format.

- Advanced crevice model: incorporated in Fluent. Important for HC emissions and accurate IC-engine simulation.

Future Direction

- Investigate the autoignition models for natural gas based on methane.
- Investigate the interaction of detailed chemistry with turbulence. Method of ISAT (*in situ* adaptive tabulation) and PDF Transport equation.
- Investigate spark ignition models for SI natural gas engines.
- Use validated models to study knock abatement strategies in practical engine geometry NETL Engine
- Develop user interface in Fluent software

Schedule/Milestones

Work Plan Schedule

Task 2.1 – Chemkin Studies/Development *(Planned Completion 09/02)*

Subtask 2.1.1 - **Compare reduced mechanisms to GRI 3.0 and select appropriate mechanisms for initial FLUENT studies *(Planned Completion 01/02)***

Subtask 2.1.2 **– Compare Chemkin Results to RCM Data/Continue feedback to Fluent Model *(Planned Completion 09/02)***

Task 2.2 - Knock Model Development *(Planned Completion 12/02)*

Subtask 2.2.1 **- Assess/Select Appropriate Ignition/Combustion Models and Incorporate into Fluent CFD Software *(Planned Completion 01/02)***

Subtask 2.2.2 **- Validate model predictions with RCM measurements and literature data *(Planned Completion 09/02)***

Subtask 2.2.3 – **Develop and Validate Crevice Model** *(Planned completion 06/02)*

Subtask 2.2.4 **- Use validated model tool to study knock abatement strategies in practical engine geometry NETL Engine and Develop User Interface *(Planned Completion 12/02)***